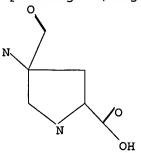
08/02/2006

Page 1

=>

Uploading C:\Program Files\Stnexp\Queries\10613961.str



chain nodes :

6 7 8 9 10 11

ring nodes : 1 2 3 4 5

chain bonds :

3-9 3-10 5-6 6-7 6-8 10-11

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 3-9 10-11

exact bonds :

2-3 3-4 3-10 4-5 5-6

normalized bonds :

6-7 6-8

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS

11:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1

STR

08/02/2006 Page 2

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 15:24:00 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 14 TO ITERATE

100.0% PROCESSED 14 ITERATIONS 8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 56 TO 504
PROJECTED ANSWERS: 8 TO 329

L2 8 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 15:24:05 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 351 TO ITERATE

100.0% PROCESSED 351 ITERATIONS 172 ANSWERS

SEARCH TIME: 00.00.01

L3 172 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 166.94 167.15

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=> s 13

L4 61 L3

=> s 14 and py<2003 22790841 PY<2003 L5 44 L4 AND PY<2003

=> s 15 and carbamate 29354 CARBAMATE 11121 CARBAMATES 34008 CARBAMATE

(CARBAMATE OR CARBAMATES)

L6 1 L5 AND CARBAMATE

=> d abs bib hitstr

L6 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

The four isomers of 4-aminopyrrolidine-2,4-dicarboxylate (APDC) were AB prepared and evaluated for their effects at glutamate receptors in vitro. (2R,4R)-APDC (2a), an aza analog of the nonselective mGluR agonist (1S, 3R) -1-aminocyclopentane-1,3-dicarboxylate ((1S, 3R) -ACPD, 1), was found to possess relatively high affinity for metabotropic glutamate receptors (mGluRs) (ACPD-sensitive [3H]glutamate binding IC50 = $6.49\pm1.21~\mu\text{M}$) with no effects on radioligand binding to NMDA, AMPA, or kainate receptors up to 100 μM . None of the other APDC isomers showed significant mGluR binding affinity, indicating that this interaction is highly stereospecific. Both 1 and 2a were effective in decreasing forskolin-stimulated cAMP formation in the adult rat cerebral cortex (EC50 = $8.17\pm2.21 \, \mu\text{M}$ for 1; EC50 = $14.51\pm5.54 \, \mu\text{M}$ for 2a); however, while 1 was also effective in stimulating basal tritiated inositol monophosphate production in the neonatal rat cerebral cortex (EC50 = $27.7\pm5.2~\mu\text{M}$), 2a (up to 100 μM) was ineffective in stimulating phosphoinositide hydrolysis in this tissue preparation, further supporting our previous observations that 2a is a highly selective agonist for mGluRs neg. coupled to adenylate cyclase. Microelectrophoretic application of either 1 or 2a to intact rat spinal neurons produced an augmentation of AMPA-induced excitation (95 \pm 10% increase for 1, 52 \pm 6% increase for 2a). Intracerebral injection of 1 (400 nmol) produced characteristic limbic seizures in mice which are not mimicked by 2a (200-1600 nmol, ic). However, the limbic seizures induced by 1 were blocked by systemically administered 2a in a dose-dependent manner (EC50 = 271 mg/kg, i.p.). It is concluded that (2R,4R)-APDC (2a) is a highly selective, systemically-active agonist of mGluRs neg. coupled to adenylate cyclase and that selective activation of these receptors in vivo can result in anticonvulsant effects.

AN 1996:383040 CAPLUS

DN 125:104243

TI Synthesis of the Four Isomers of 4-Aminopyrrolidine-2,4-dicarboxylate: Identification of a Potent, Highly Selective, and Systemically-Active Agonist for Metabotropic Glutamate Receptors Negatively Coupled to Adenylate Cyclase

AU Monn, James A.; Valli, Matthew J.; Johnson, Bryan G.; Salhoff, Craig R.; Wright, Rebecca A.; Howe, Trevor; Bond, Ann; Lodge, David; Spangle, Larry A.; et al.

CS Core Technology Division, Eli Lilly and Company, Indianapolis, IN, USA

SO Journal of Medicinal Chemistry (1996), 39(15), 2990-3000 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

OS CASREACT 125:104243

IT 169209-63-6P, (2R,4R)-4-Aminopyrrolidine-2,4-dicarboxylate
171336-79-1P 171336-80-4P 171336-81-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis of four isomers of 4-aminopyrrolidine-2,4-dicarboxylate as agonists for metabotropic glutamate receptors neg. coupled to adenylate cyclase)

RN 169209-63-6 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-, (2R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

$$HO_2C$$
 R
 R
 H_2N
 CO_2H

RN 171336-79-1 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-, (2S-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

$$HO_2C$$
 S
 H_2N
 CO_2H

RN 171336-80-4 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-, (2S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$HO_2C$$
 S
 R
 CO_2H

RN 171336-81-5 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-, (2R-trans)- (9CI) (CA INDEX

NAME)

Absolute stereochemistry. Rotation (+).

$$HO_2C$$
 R
 S
 CO_2H

1516378 GROUP

988533 GROUPS

2120181 GROUP

(GROUP OR GROUPS)

15139 PROTECTING GROUP

(PROTECTING (W) GROUP)

1 L5 AND PROTECTING GROUP

=> d 17 not 16

L6 IS NOT VALID HERE

For an explanation, enter "HELP DISPLAY".

=> d abs 17

L7

L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN GI

The present invention provides pyrrolidinyl dicarboxylic acid derivs. I wherein: R1 and R2 are each individually H or a carboxy protecting group; R4 is H or an amino protecting group;
R3 = e.g., C1-16 alkyl, C3-8 cycloalkyl; C3-8 cycloalkenyl, aryl, that affect certain excitatory amino acid receptors (no data), and are useful in the treatment of neurol. disorders and psychiatric disorders. This invention further provides novel pyrrolidinyl di-carboxylic acid derivs. and pharmaceutical formulations employing these novel compds. Thus, cis-4-hydroxy-D-proline was esterified and N-benzylated to provide (2R,4R) Et 1-benzyl-4-hydroxypyrrolidine-2-carboxylate; this was oxidized to the 4-oxo derivative which was treated with KCN/ammonium carbonate to afford (2R,4R) di-Et 1-benzyl-4-aminopyrrolidine-2,4-dicarboxylate; the latter

was N-protected and debenzylated to afford (2R,4R) di-Et 4-(BOC-amino)pyrrolidine-2,4-dicarboxylate (II) as the scaffold intermediate. Reductive alkylation of II with pentanal afforded (2R,4R) di-Et 4-(BOC-amino)-1-pentylpyrrolidine-2,4-dicarboxylate which was deprotected and hydrolyzed to (2R,4R) 4-amino-1-pentylpyrrolidine-2,4dicarboxylic acid (I; R1 = R2 = R4 = H, R3 = pentyl).

Page 6

=> d abs fbib hitstr

L7ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN GΙ

AB The present invention provides pyrrolidinyl dicarboxylic acid derivs. I wherein: R1 and R2 are each individually H or a carboxy protecting group; R4 is H or an amino protecting group; R3 = e.g., C1-16 alkyl, C3-8 cycloalkyl; C3-8 cycloalkenyl, aryl, that affect certain excitatory amino acid receptors (no data), and are useful in the treatment of neurol. disorders and psychiatric disorders. This invention further provides novel pyrrolidinyl di-carboxylic acid derivs. and pharmaceutical formulations employing these novel compds. Thus, cis-4-hydroxy-D-proline was esterified and N-benzylated to provide (2R,4R) Et 1-benzyl-4-hydroxypyrrolidine-2-carboxylate; this was oxidized to the 4-oxo derivative which was treated with KCN/ammonium carbonate to afford (2R,4R) di-Et 1-benzyl-4-aminopyrrolidine-2,4-dicarboxylate; the latter was N-protected and debenzylated to afford (2R,4R) di-Et 4-(BOC-amino)pyrrolidine-2,4-dicarboxylate (II) as the scaffold intermediate. Reductive alkylation of II with pentanal afforded (2R,4R) di-Et 4-(BOC-amino)-1-pentylpyrrolidine-2,4-dicarboxylate which was deprotected and hydrolyzed to (2R,4R) 4-amino-1-pentylpyrrolidine-2,4dicarboxylic acid (I; R1 = R2 = R4 = H, R3 = pentyl). AN 1996:410401 CAPLUS

DN 125:86486

ΤI (2R,4R)-4-Aminopyrrolidine-2,4-dicarboxylic acid derivatives as metabotropic glutamate receptor antagonists

TN Monn, James Allen; Tizzano, Joseph Patrick; Valli, Matthew J.

PA Eli Lilly and Co., USA

SO PCT Int. Appl., 97 pp. CODEN: PIXXD2

DTPatent

LΑ English

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE ----_____ -----PΙ WO 9605828 **A1** 19960229 WO 1995-US10320 19950814 <--W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD,

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MARPAT 125:86486
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OS

TT 178415-98-0P

CN

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((2R,4R)-4-aminopyrrolidine-2,4-dicarboxylic acid derivs. as metabotropic glutamate receptor antagonists)

RN178415-98-0 CAPLUS

> 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(3,3-diphenylpropyl)-, (2R,4R) - (9CI) (CA INDEX NAME)

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TT
    171336-76-8P 178415-42-4P 178415-44-6P
     178415-46-8P 178415-48-0P 178415-50-4P
     178415-52-6P 178415-54-8P 178415-56-0P
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    178416-07-4P 178416-09-6P 178416-11-0P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        ((2R,4R)-4-aminopyrrolidine-2,4-dicarboxylic acid derivs. as
```

metabotropic glutamate receptor antagonists)

RN 171336-76-8 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(phenylmethyl)-, (2R,4R)(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 178415-42-4 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-pentyl-, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$(CH_2)_4$$
 $(CH_2)_4$
 R
 R
 CO_2H
 R
 R

RN 178415-44-6 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(3-phenylpropyl)-, (2R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-46-8 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(2,2-dimethylpropyl)-, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-48-0 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-propyl-, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-50-4 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(2,2-diphenylethyl)-, (2R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-52-6 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-butyl-, (2R-cis)- (9CI) (CA INDEX NAME)

RN 178415-54-8 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(cyclohexylmethyl)-, (2R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-56-0 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(2-phenylethyl)-, (2R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-58-2 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(4-phenylbutyl)-, (2R-cis)-(9CI) (CA INDEX NAME)

$$(CH_2)_4$$
 Ph
 R CO_2H
 R R

RN 178415-60-6 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(5-phenylpentyl)-, (2R-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$(CH_2)_5$$
 Ph
 R CO_2H
 R R

RN 178415-62-8 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(2-naphthalenylmethyl)-, (2R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-64-0 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-([1,1'-biphenyl]-4-ylmethyl)-, (2R,4R)- (9CI) (CA INDEX NAME)

08/02/2006

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RN 178415-66-2 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-([1,1'-biphenyl]-2-ylmethyl)-, (2R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-68-4 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[[4-(phenylmethoxy)phenyl]methyl]-, (2R-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-70-8 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[(2-iodophenyl)methyl]-,

(2R-cis) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-72-0 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[(4-dodecylphenyl)methyl]-, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$N$$
 R
 CO_2H
 R
 NH_2

RN 178415-74-2 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[(6,7-dimethoxy-2-oxo-2H-1-benzopyran-4-yl)methyl]-, (2R-cis)- (9CI) (CA INDEX NAME)

RN 178415-76-4 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[(3,4-dichlorophenyl)methyl]-, (2R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$C1$$
 $C1$
 R
 R
 $C0_2H$
 R
 R

RN 178415-78-6 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[(2,6-dichlorophenyl)methyl]-, (2R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-80-0 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[[3,4-bis(phenylmethoxy)phenyl]methyl]-, (2R-cis)- (9CI) (CA INDEX NAME)

RN 178415-82-2 CAPLUS
CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[[4-(2-phenylethenyl)phenyl]methyl]-, [2R-[1(E),2α,4α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 178415-84-4 CAPLUS
CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[[2-(trifluoromethyl)phenyl]methyl]-, (2R-cis)- (9CI) (CA INDEX NAME)

RN 178415-86-6 CAPLUS
CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[[2-

[(phenylsulfonyl)methyl]phenyl]methyl]-, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-88-8 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(1-naphthalenylmethyl)-, (2R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-90-2 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(diphenylmethyl)-, (2R,4R)-

(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-92-4 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[(4-chlorophenyl)methyl]-, (2R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$N$$
 R
 CO_2H
 R
 NH_2

RN 178415-94-6 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[(3-chlorophenyl)methyl]-, (2R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178415-96-8 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-[(2-chlorophenyl)methyl]-,

(2R,4R) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178416-00-7 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-/(1-oxo-3,3-diphenylpropyl)-, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178416-01-8 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(diphenylacetyl)-, (2R-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178416-03-0 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(1-oxo-3-phenylpropyl)-, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178416-05-2 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(cyclohexylcarbonyl)-, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178416-07-4 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(phenylacetyl)-, (2R-cis)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 178416-09-6 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-(1-oxo-3-phenyl-2-propenyl)-, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 178416-11-0 CAPLUS

CN 2,4-Pyrrolidinedicarboxylic acid, 4-amino-1-benzoyl-, (2R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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L1 STRUCTURE UPLOADED

L2 8 S L1 L3 172 S L1 FUL 08/02/2006 Page 21

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L4 61 S L3

L5 44 S L4 AND PY<2003 L6 1 S L5 AND CARBAMATE

L7 1 S L5 AND PROTECTING GROUP

FILE 'STNGUIDE' ENTERED AT 15:29:33 ON 08 FEB 2006

=> s 14 and ?fluorenyl?

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answer sets from structure searches can be used in crossover searches
and can be combined with text terms.

=> s 14 and fluorenyl

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
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structure-building or screen commands and text search terms. L#s
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structures files separately from text terms or profiles. The L#
answer sets from structure searches can be used in crossover searches
and can be combined with text terms.

=> s 15 and fluorenyl

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID
The query entered contains both search terms created by
structure-building or screen commands and text search terms. L#s
created via the STRUCTURE or SCREEN commands must be searched in the
structures files separately from text terms or profiles. The L#
answer sets from structure searches can be used in crossover searches
and can be combined with text terms.

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FULL ESTIMATED COST	ENTRY 0.78	SESSION 191.69
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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http://www.cas.org/infopolicy.html

=> s 15 and fluorenyl

4084 FLUORENYL

5 FLUORENYLS

4085 FLUORENYL

(FLUORENYL OR FLUORENYLS)

L8 0 L5 AND FLUORENYL

=> s 15 and fluorenyl?

9942 FLUORENYL?

L9 0 L5 AND FLUORENYL?